

## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	725	cetomacrogol	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/29 11:55
L2	292	L1 and glycerol and talc and cellulose	US-PGPUB; USPAT	NEAR	ON	2006/08/29 12:04
L3	55	I2 and menthol	US-PGPUB; USPAT	NEAR	ON	2006/08/29 11:56
L4	49	I3 and (paraffin or (acetyl alcohol) or (propylene glycol))	US-PGPUB; USPAT	NEAR	ON	2006/08/29 11:57
L6	30	I4 and @ad<"20040416"	US-PGPUB; USPAT	NEAR	ON	2006/08/29 12:06
L7	29	I6 and (fung\$ or bacter\$ or antibacter\$ or disinfect\$)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/29 12:06
L8	4	I7 and cosmet\$	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/29 12:02
L9	74	I2 and ((methyl or ethyl) (cellulose))	US-PGPUB; USPAT	NEAR	ON	2006/08/29 12:06
L10	2	I9 and I6	US-PGPUB; USPAT	NEAR	ON	2006/08/29 12:05
L11	48	I9 and (fung\$ or bacter\$ or antibacter\$ or disinfect\$)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/29 12:06
L12	15	I11 and @ad<"20040416"	US-PGPUB; USPAT	NEAR	ON	2006/08/29 12:06
S1	1	((JANUSZ) near2 (MARCINKIEWICZ)).INV.	US-PGPUB; USPAT	NEAR	ON	2006/08/29 11:54
S2	2	taurine ADJ bromamine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/23 17:59

## EAST Search History

S3	2	taur\$ ADJ bromam\$	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/23 17:42
S4	18	taurine ADJ chloramine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 15:53
S5	2	("3998945").PN.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	OFF	2006/08/25 17:24
S6	0	S5 and taurine bromamine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:24
S7	1	S5 and taurine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:26
S8	2	"3932605" and taurine	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:29
S9	1646	aminoethanesulfonic acid	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:29
S10	623	S9 and (fung\$ or bacter\$ or antibacter\$ or disinfect\$)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/29 11:59

## EAST Search History

S11	0	S9 and ((fung\$ or bacter\$ or antibacter\$ or disinfect\$) NEAR5 aminoethanesulfonic)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:31
S12	0	((fung\$ or bacter\$ or antibacter\$ or disinfect\$) NEAR5 aminoethanesulfonic)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:31
S13	0	((fung\$ or bacter\$ or antibacter\$ or disinfect\$) NEAR10 aminoethanesulfonic)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:31
S14	1	((fung\$ or bacter\$ or antibacter\$ or disinfect\$) NEAR20 aminoethanesulfonic)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/25 17:32
S16	2	("4772592").PN.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	OFF	2006/08/28 14:08
S17	0	taurine ADJ acne	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 14:21
S18	18	(taurine ADJ chloramine) or (ethanesulfonic NEAR3 (Bromoamino or chloroamino))	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 15:57
S19	52	(taurine ADJ chloramine) or (ethanesulfonic NEAR3 (Bromoamino or chloroamino) or (chlorotaurine or bromotaurine))	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:52

## EAST Search History

S20	19	S19 and (cellulose or cetomakrogel or glycerol or acne or methylcellulose or ethylcellulose or menthol)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 17:25
S21	338	ceto?	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 18:02
S22	0	S21 and estolate	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 18:02
S23	1824	estolate	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 18:02
S24	338	ceto?	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 18:51
S25	18	cetomacrogel or cetomakrogel	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 18:53
S26	725	(cetomacrogel or cetomakrogel)	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:11
S27	725	cetomacrogel	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:12

## EAST Search History

S28	15	S27 and estolate	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:12
S29	0	EP1239853	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:55
S30	0	EP20010965273	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:55
S31	10	GOTTARDI WALDEMAR	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	NEAR	ON	2006/08/28 19:55

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=> d his

(FILE 'HOME' ENTERED AT 11:36:39 ON 29 AUG 2006)

FILE 'HCAPLUS' ENTERED AT 11:36:55 ON 29 AUG 2006

FILE 'REGISTRY' ENTERED AT 11:37:01 ON 29 AUG 2006

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 13 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:38:06 ON 29 AUG 2006

L4 177 S L3

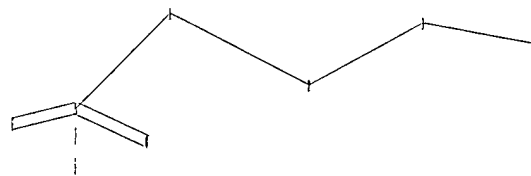
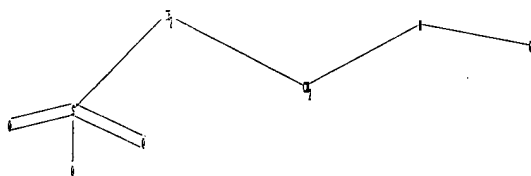
L5 156 S L4 AND 1800<=PY<=2004

L6 42 S L4 AND (DISINFECT? OR ANTIMICROB? OR ANTIBACT? OR BACTERIA OR

L7 33 S L6 AND L5

L8 1 S L7 AND (GLYCEROL OR ACNE OR CELLULOSE OR CETOMAKROGEL OR CETO

FILE 'HOME' ENTERED AT 11:44:31 ON 29 AUG 2006



chain nodes :  
1 2 3 4 5 6 7 8  
chain bonds :  
1-2 1-5 2-3 3-4 5-6 5-7 5-8  
exact/norm bonds :  
3-4 5-6 5-7 5-8  
exact bonds :  
1-2 1-5 2-3

G1:Cl,Br,F,I

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L1 STRUCTURE UPLOADED

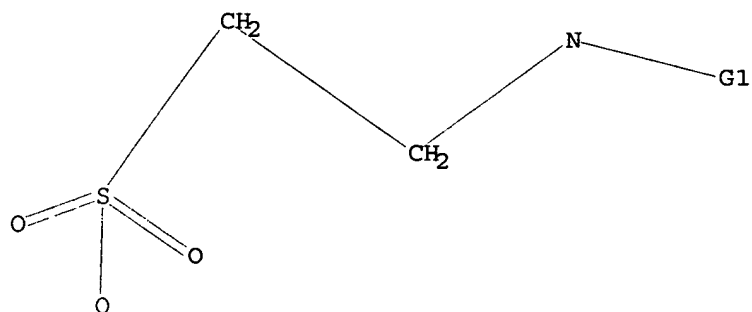
=> d l1  
L1 HAS NO ANSWERS

29/08/2006

Roy P. Issac 10/825,288

L1

STR



G1 Cl,Br,F,I

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 11:37:39 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1 TO 80

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 11:37:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS

13 ANSWERS

SEARCH TIME: 00.00.01

L3 13 SEA SSS FUL L1

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

167.38

170.12

FILE 'CAPLUS' ENTERED AT 11:38:06 ON 29 AUG 2006

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=> s l3

L4 177 L3

=> d ibib abs hitstr 1

L4 ANSWER 1 OF 177 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:768656 CAPLUS

TITLE: N-halogenated and N,N-dihalogenated amino acids in combination with hypohalous acids for use as antimicrobial agents

INVENTOR(S): Najafi, Ramin; Bassiri, Mansour; Wang, Lu; Khosrovi, Behzad

PATENT ASSIGNEE(S): Novacal Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 72pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006081392	A1	20060803	WO 2006-US2875	20060125
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: US 2005-647366P P 20050125

AB The invention relates to pharmaceutical compns. comprising amino acids A-CR0R1-R-(CH2)0-13-C(Y)(Z)-X' [A is H, mono- or dihaloamino; R is a single bond or C3-C6 cycloalkylene; R0 is H or alkyl; R1 is H, alkyl or CO2H; or R0R1C is C3-C6 cycloalkyl; Y is H, alkyl, NH2, mono- or dihaloamino; Z is H or alkyl; X' is H, CO2H, CONH2, SO3H, SO2NH2, PO3H2 or B(OH)2; the R or CH2 groups may be substituted by mono- or dihaloamino] or their pharmaceutically-acceptable derivs. in combination with hypohalous acids or salts which have antibacterial, anti-infective, antimicrobial, sporicidal, disinfectant, antifungal and antiviral properties. Thus, a 1:1 isotonic mixture of Cl2NCH2CMe2SO3H (prepared by N-chlorination) and hypochlorous has a synergistic antiviral effect against Adenovirus, when compared against the antiviral effect of hypochlorous acid or

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Cl<sub>2</sub>NCH<sub>2</sub>CMe<sub>2</sub>SO<sub>3</sub>H alone.

IT 51036-13-6P 83152-69-6P 162069-44-5P  
846056-91-5P 903893-41-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(N-halogenated and N,N-dihalogenated amino acids in combination with  
hypohalous acids for use as antimicrobial agents)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino) - (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

RN 83152-69-6 CAPLUS

CN Ethanesulfonic acid, 2-(dichloroamino) - (9CI) (CA INDEX NAME)

Cl<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

RN 162069-44-5 CAPLUS

CN Ethanesulfonic acid, 2-(dibromoamino) - (9CI) (CA INDEX NAME)

Br<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

RN 846056-91-5 CAPLUS

CN Ethanesulfonic acid, 2-(diiodoamino) - (9CI) (CA INDEX NAME)

I<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

RN 903893-41-4 CAPLUS

CN Ethanesulfonic acid, 2-(iodoamino) - (9CI) (CA INDEX NAME)

INH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> S L4 AND 1800<=PY<=2004

24958388 1800<=PY<=2004

L5 156 L4 AND 1800<=PY<=2004

=> S L4 AND (DISINFECT? OR ANTIMICROB? OR ANTIBACT? OR BACTERIA OR FUNG? OR COSMET?)

99577 DISINFECT?

66518 ANTIMICROB?

89224 ANTIBACT?

304249 BACTERIA

100 BACTERIAS

304304 BACTERIA

(BACTERIA OR BACTERIAS)

219645 FUNG?

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78255 COSMET?

L6 42 L4 AND (DISINFECT? OR ANTIMICROB? OR ANTIBACT? OR BACTERIA OR FUNG?  
OR COSMET?)

=> l6 and l5

L6 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (=>).

=> s l6 and l5

L7 33 L6 AND L5

=> S L7 AND (GLYCEROL OR ACNE OR CELLULOSE OR CETOMAKROGEL OR CETOMACROGOL OR  
MENTHOL)

134355 GLYCEROL

1311 GLYCEROLS

134817 GLYCEROL

(GLYCEROL OR GLYCEROLS)

5811 ACNE

1454 ACNES

6852 ACNE

(ACNE OR ACNES)

342364 CELLULOSE

4302 CELLULOSES

342854 CELLULOSE

(CELLULOSE OR CELLULOSES)

0 CETOMAKROGEL

221 CETOMACROGOL

1 CETOMACROGOLS

221 CETOMACROGOL

(CETOMACROGOL OR CETOMACROGOLS)

11834 MENTHOL

252 MENTHOLS

11886 MENTHOL

(MENTHOL OR MENTHOLS)

L8 1 L7 AND (GLYCEROL OR ACNE OR CELLULOSE OR CETOMAKROGEL OR  
CETOMACROGOL OR MENTHOL)

=> DIS L8 1 TI

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

TI Method using taurine bromamine for inhibiting pathogenic bacteria  
and fungi growth, and microbicidal composition

=> d l7 ibib abs hitstr 1-10

L7 ANSWER 1 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1034828 CAPLUS

DOCUMENT NUMBER: 142:215967

TITLE: Hypochlorous acid and taurine-N-monochloramine in  
periodontal diseases

AUTHOR(S): Mainnemare, A.; Megarbane, B.; Soueidan, A.; Daniel,  
A.; Chapple, I. L. C.

CORPORATE SOURCE: Service de Parodontologie, UFR d'Odontologie, Nantes,  
44 042, Fr.

SOURCE: Journal of Dental Research (2004), 83(11),  
823-831

CODEN: JDREAF; ISSN: 0022-0345

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PUBLISHER: International Association for Dental Research  
DOCUMENT TYPE: Journal; General Review  
LANGUAGE: English

AB A review. Chronic periodontitis is a multi-factorial disease involving anaerobic bacteria and the generation of an inflammatory response, including the production of metalloproteinases, proinflammatory cytokines, and eicosanoids. Hypochlorous acid (HOCl) and taurine-N-monochloramine (TauCl) are the end-products of the neutrophilic polymorphonuclear leukocyte (PMN) respiratory burst. They act synergistically to modulate the inflammatory response. In the extracellular environment, HOCl and TauCl may directly neutralize interleukin 6 (IL-6) and several metalloproteinases, while HOCl increases the capacity of  $\alpha$ 2-macroglobulin to bind Tumor Necrosis Factor- $\alpha$ , IL-2, and IL-6, and facilitates the release of various growth factors. TauCl inhibits the production of inflammatory mediators, prostaglandins, and nitric oxide. HOCl activates tyrosine kinase signaling cascades, generating an increase in the production of extracellular matrix components, growth factors, and inflammatory mediators. Thus, HOCl and TauCl appear to play a crucial role in the periodontal inflammatory process. Taken together, these findings may offer opportunities for the development of novel host-modulating therapies for the treatment of periodontitis.

IT 51036-13-6, Taurine chloramine  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(hypochlorous acid and taurine-N-monochloramine interaction with inflammatory mediators in periodontal diseases)

RN 51036-13-6 CAPLUS  
CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:905635 CAPLUS

DOCUMENT NUMBER: 141:374694

TITLE: Method using taurine bromamine for inhibiting pathogenic bacteria and fungi growth, and microbicidal composition

INVENTOR(S): Marcinkiewicz, Janusz; Kasprowicz, Andrzej

PATENT ASSIGNEE(S): Pol.

SOURCE: U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004214891	A1	20041028	US 2004-825288	20040416 <--
WO 2004093853	A2	20041104	WO 2004-PL27	20040420 <--
WO 2004093853	A3	20060330		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,  
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,  
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,  
TD, TG

EP 1663195 A2 20060607 EP 2004-728482 20040420

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

PRIORITY APPLN. INFO.:

PL 2003-359792 A 20030422  
PL 2004-367052 A 20040407  
WO 2004-PL27 W 20040420

AB In a method for inhibiting pathogenic bacteria and fungi  
growth, bacteria and fungi are treated with an  
effective quantity of taurine bromamine,. The effective quantity of  
taurine bromamine has concns. of 10-100 weight%. The microbicidal  
composition, of  
the invention contains taurine bromamine in concns. of 10-100 weight%.

IT 52316-57-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(taurine bromamine for inhibiting pathogenic bacteria and  
fungi growth, and microbicidal composition)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L7 ANSWER 3 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:419602 CAPLUS

DOCUMENT NUMBER: 141:156025

TITLE: Down-regulatory effect of N-chlorotaurine on  
tryptophan degradation and neopterin production in  
human PBMC

AUTHOR(S): Wirleitner, Barbara; Neurauter, Gabriele; Nagl,  
Markus; Fuchs, Dietmar

CORPORATE SOURCE: Institute of Medical Chemistry and Biochemistry,  
Medical University of Innsbruck, Innsbruck, A-6020,  
Austria

SOURCE: Immunology Letters (2004), 93(2-3), 143-149

CODEN: IMLED6; ISSN: 0165-2478

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-Chlorotaurine (NCT) plays an important role in the human defense system  
as a main component of long-lived oxidants, and shows bactericidal,  
fungicidal, and virucidal activity. Besides this role, NCT seems  
to act regulatory on immunocompetent cells by altering cytokine production  
NCT inhibited nitric oxide, TNF- $\alpha$ , and prostaglandin E<sub>2</sub> (PGE<sub>2</sub>)  
production in activated rodent macrophages, and suppressed superoxide anion,  
IL-6, and IL-8 formation in human polymorphonuclear leukocytes. In this  
study, the influence of NCT on the production of neopterin and the activation  
of the enzyme indoleamine-2,3 dioxygenase (IDO) was investigated in human  
peripheral blood mononuclear cells (PBMC). Both events are well  
established to be triggered by IFN- $\gamma$  and therefore related to  
Th1-type immune activation. Mitogen-induced neopterin production as well as

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tryptophan degradation were drastically reduced upon addition of NCT. Results fit in the concept of a reduction of pro-inflammatory cytokines by this compound

In contrast to earlier results, where NCT was suggested to act primarily down-regulatory on Th2 cells, the authors propose also a strong suppressive effect of NCT on Th1-type immunity.

IT 51036-13-6, N-Chlorotaurine

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(effect of chlorotaurine on tryptophan degradation and neopterin production in human mononuclear cells)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:095773 CAPLUS

DOCUMENT NUMBER: 139:371812

TITLE: Tolerability and efficacy of N-chlorotaurine in comparison with chloramine T for the treatment of chronic leg ulcers with a purulent coating: a randomized phase II study

AUTHOR(S): Nagl, M.; Nguyen, V. A.; Gottardi, W.; Ulmer, H.; Hopfl, R.

CORPORATE SOURCE: Institute of Hygiene and Social Medicine, Leopold-Franzens-University of Innsbruck, Innsbruck, A-6010, Austria

SOURCE: British Journal of Dermatology (2003), 149(3), 590-597

CODEN: BJDEAZ; ISSN: 0007-0963

PUBLISHER: Blackwell Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The well-known active chlorine compound chloramine T (CAT) with broad-spectrum antimicrobial activity is in common therapeutic use for leg ulcers with purulent coatings; however, this treatment is painful. The tolerability of the less aggressive N-chlorotaurine (NCT), an endogenous compound also produced in vivo by stimulated human granulocytes, could be superior. The aim was to assess the tolerability and efficacy of NCT in the cleaning of purulent coatings in chronic leg ulcers in comparison with CAT. In a double-blind, randomized phase IIb clin. study 40 patients were treated for a median of 7 days (range 3-14) with a 1% aqueous solution of either NCT (20 subjects) or CAT (20 subjects) by twice-daily application of dressings soaked in the test solns. Criteria for evaluation of tolerability were intensity and duration of pain caused by the ulcer therapy and scores of tissue toxicity (necrosis, granulation tissue and re-epithelialization). Therapeutic efficacy was graded as scores of intensity of purulent coating of the ulcers. The concentration tolerated in vitro by human epidermoid carcinoma cells was at least 10-fold higher for NCT (0.01%) compared with CAT (0.0001.0001%). There was significantly less pain caused by NCT compared with CAT ( $P < 0.05$ ) on days 1 and 4 and a trend for a shorter duration of pain ( $P = 0.093$ ). The scores of intensity of coating improved without difference in both treatment groups, whereas granulation and re-epithelialization appeared

earlier in the NCT group ( $P < 0.05$ ). Non-quant. microbiol. cultures from ulcer smears revealed persistence of colonization by bacterial species in approx. half of both treatment groups. Conclusions Both active chlorine compds. were helpful in reducing purulent coatings. Because of its lower toxicity and better tolerability, NCT is of advantage in the treatment of leg ulcers.

IT 51036-13-6, N-Chlorotaurine  
 RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (N-chlorotaurine vs. chloramine T for treatment of chronic leg ulcers with purulent coating)  
 RN 51036-13-6 CAPLUS  
 CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:SC0020 CAPLUS

DOCUMENT NUMBER: 138:200400

TITLE: Chemical properties of N-chlorotaurine sodium, a key compound in the human defence system

AUTHOR(S): Gottardi, Waldemar; Nagl, Markus

CORPORATE SOURCE: Institute for Hygiene and Social Medicine, Medical Faculty, University of Innsbruck, Innsbruck, A 6010, Austria

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2002), 335(9), 411-421

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-Chlorotaurine (NCT) is known to play an important role in the human defense system. The already proved utility of the sodium salt as a disinfectant in human medicine suggested a thorough investigation of its chemical properties. Chlorine transfer to N-H groups (transhalogenation) and oxidation of thio and aromatic compds. represent its main reactions. Auto-chlorination causes disproportionation forming N,N-dichlorotaurine (NDCT) with  $K_d = [\text{NDCT}][\text{taurine}]/[\text{NCT}]^2 \text{ aH}^+ = (4.5 \pm 0.8) \times 10^6$ , while the reaction with ammonium releasing  $\text{NH}_2\text{Cl}$  is characterized by  $K_{\text{NHCl}_2} = [\text{NH}_2\text{Cl}][\text{taurine}]/[\text{NCT}][\text{NH}_4^+] \text{ fa}_2 = 0.02 \pm 0.004$ . The verified unique stability and low-level reactivity of NCT are considered essential for its function in the mammalian defense system and its practical applicability, which manifests itself in an optimal compromise between microbicidal activity and toxicity.

IT 144557-26-6, N-Chlorotaurine sodium  
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (chemical properties of N-chlorotaurine sodium, key compound in human defense system)  
 RN 144557-26-6 CAPLUS  
 CN Ethanesulfonic acid, 2-(chloroamino)-, monosodium salt (9CI) (CA INDEX NAME)

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ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

● Na

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:574922 CAPLUS

DOCUMENT NUMBER: 137:119639

TITLE: Use of halogenated compositions as antiseptic and antiinflammatory agents

INVENTOR(S): Mainnemare, Arnaud

PATENT ASSIGNEE(S): Fr.

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT NO. 2002:574922

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058692	A2	20020801	WO 2002-FR151	20020116 <--
WO 2002058692	C2	20030306		
WO 2002058692	A3	20031224		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
FR 2819723	A1	20020726	FR 2001-862	20010123 <--
CA 2435419	AA	20020801	CA 2002-2435419	20020116 <--
AU 2002231889	A1	20020806	AU 2002-231889	20020116 <--
EP 1401422	A2	20040331	EP 2002-711967	20020116 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004519462	T2	20040702	JP 2002-559026	20020116 <--
US 2004022871	A1	20040205	US 2003-622262	20030718 <--
PRIORITY APPLN. INFO.:			FR 2001-862	A 20010123
			WO 2002-FR151	W 20020116

AB The invention concerns pharmaceutical compns. comprising (i) at least a halogenated composition and (ii) at least a N-halogenated derivative of at least a compound selected among zwitterion and/or amino acid compds. The halogenated composition is advantageously an alkaline metal hypochlorite, and preferably sodium hypochlorite, and N-halogenated derivative is preferably a N-halogenated taurine derivative and particularly a N-haloamine taurine derivative and more preferably still N-chloramine taurine. The invention also concerns the preparation of said compns. and their use as very large spectrum

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antiseptic, anti-inflammatory agent and as immunity modulator, without stimulating myeloperoxidase activity. Sodium hypochlorite is used at a concentration of 0.2 mol/L in odontol. (no data).

IT 51036-13-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(use of halogenated compns. as antiseptic and antiinflammatory agents)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

L7 ANSWER 7 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:537188 CAPLUS

DOCUMENT NUMBER: 137:123906

TITLE: Oxidation of I $\kappa$ B $\alpha$  at methionine 45 is one cause of taurine chloramine-induced inhibition of NF- $\kappa$ B activation

AUTHOR(S): Kanayama, Atsuhiko; Inoue, Jun-Ichiro; Sugita-Konishi, Yoshioko; Shimizu, Makoto; Miyamoto, Yusei

CORPORATE SOURCE: Department of Applied Biological Chemistry, Graduate School of Agricultural and Life Sciences, University of Tokyo, Tokyo, 113-8657, Japan

SOURCE: Journal of Biological Chemistry (2002), 277(27), 24049-24056

CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A band shift of I $\kappa$ B $\alpha$  was observed in Western blots with Jurkat cells treated with 1 mM taurine chloramine (TauCl) for 1 h. TauCl treatment inhibited tumor necrosis factor  $\alpha$  (TNF $\alpha$ )-initiated nuclear factor  $\kappa$ B (NF- $\kappa$ B) activation. TauCl did not inhibit either the upstream of I $\kappa$ B kinase (IKK) activation or IKK itself but did inhibit NF- $\kappa$ B activation induced by IKK overexpression. Deletion expts. showed that a TauCl modification site causing the band shift of I $\kappa$ B $\alpha$  is Met45. High performance liquid chromatog. and mass spectrometry analyses of a small peptide containing Met45 revealed that TauCl oxidizes Met45. A mutant of I $\kappa$ B $\alpha$  whose Met45 was converted to alanine did not generate a band shift upon TauCl treatment and degraded in response to TNF $\alpha$  stimulation. However, a reporter assay revealed that NF- $\kappa$ B-dependent luciferase expression was not fully recovered in cells transfected with this mutant. These results indicate that Met45 oxidation of I $\kappa$ B $\alpha$  is a mol. mechanism underlying the TauCl-induced inhibition of NF- $\kappa$ B activation. A similar band shift was observed when HL-60 cells expressing myeloperoxidase were treated with 100  $\mu$ M hydrogen peroxide for 5 min. When rat neutrophils were incubated with bacteria, intracellular taurine decreased interleukin-8 production. Therefore, taurine may help suppress excessive inflammatory reaction in neutrophils.

IT 51036-13-6, Taurine chloramine

RL: BSU (Biological study, unclassified); BIOL (Biological study) (oxidation of I $\kappa$ B $\alpha$  at methionine 45 is one cause of taurine chloramine-induced inhibition of NF- $\kappa$ B activation)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

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ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:414549 CAPLUS

DOCUMENT NUMBER: 137:106404

TITLE: Impact of N-chlorotaurine on viability and production of secreted aspartyl proteinases of Candida spp.

AUTHOR(S): Nagl, Markus; Gruber, Andreas; Fuchs, Anita; Lell, Claudia P.; Lemberger, Eva-Maria; Zepelin, Margarete Borg-Von; Wurzner, Reinhard

CORPORATE SOURCE: Institute of Hygiene and Social Medicine, Leopold-Franzens-University of Innsbruck, Innsbruck, A-6010, Austria

SOURCE: Antimicrobial Agents and Chemotherapy (2002), 46(6), 1996-1999

CODEN: AMACCO; ISSN: 0066-4804

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-chlorotaurine, an endogenous long-lived oxidant, demonstrated fungicidal activity against Candida spp. and a potent antifungal effect. Secreted aspartyl proteinases, important fungal virulence factors, proved to be a first target of impact. These results provide support for the topical application of N-chlorotaurine as an antimicrobial agent in yeast infections.

IT 51036-13-6, N-Chlorotaurine

RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(N-chlorotaurine antifungal effects on viability and aspartyl proteinase of Candida)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:275784 CAPLUS

DOCUMENT NUMBER: 136:299677

TITLE: Chloramines as antiviral agents for sterilization of blood

INVENTOR(S): Fliss, Henry

PATENT ASSIGNEE(S): University of Ottawa, Can.

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028384	A1	20020411	WO 2001-CA1421	20011005 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2322564	AA	20020406	CA 2000-2322564	20001006 <--
AU 2001095326	A5	20020415	AU 2001-95326	20011005 <--
PRIORITY APPLN. INFO.:			CA 2000-2322564	A 20001006
			WO 2001-CA1421	W 20011005

AB The present invention provides for the use of chloramines formed from hypochlorous acid and an amine-containing compound as antiviral agents and as sterilizing agents for blood. The chloramines are active against viruses, including retroviruses, having cysteine-rich regions. Such viruses include HIV. The preferred chloramine is taurine-chloramine. The chloramines may be used as a sterilizing agent for blood and blood products including whole blood, packed red blood cells, and serum, and may be used in vitro, or ex vivo.

IT 51036-13-6P, Taurine chloramine  
 RL: POC (Pharmacological activity); SPN (Synthesis preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(chloramines as antiviral agents for sterilization of blood)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:220365 CAPLUS

DOCUMENT NUMBER: 136:241630

TITLE: Fungicidal agent containing N-chlorotaurine and use thereof

INVENTOR(S): Gottardi, Waldemar; Nagl, Markus; Neher, Andreas

PATENT ASSIGNEE(S): Austria

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022118	A1	20020321	WO 2001-EP10437	20010910 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR,				

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TT, UA, UG, US, UZ, VN, YU, ZW  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
AU 2001085944 A5 20020326 AU 2001-85944 20010910 <--  
EP 1239853 A1 20020918 EP 2001-965273 20010910 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
US 2004116521 A1 20040617 US 2004-380414 20040202 <--  
PRIORITY APPLN. INFO.: DE 2000-10045868 A 20000914  
WO 2001-EP10437 W 20010910  
AB A fungicidal agent for treating infectious diseases caused by  
fungi contains N-chlorotaurine or one of its salts in aqueous solution,  
optionally with usual additives.  
IT 51036-13-6, N-Chlorotaurine 144557-26-6  
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical  
process); THU (Therapeutic use); BIOL (Biological study); PROC (Process);  
USES (Uses)  
(fungicidal agent containing N-chlorotaurine)  
RN 51036-13-6 CAPLUS  
CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

51 144557-26-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)-, monosodium salt (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

● Na

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> D COST

COST IN U.S. DOLLARS

	SINCE FILE	TOTAL
	ENTRY	SESSION
CONNECT CHARGES	4.00	7.38
NETWORK CHARGES	0.60	0.84
SEARCH CHARGES	25.35	191.85
DISPLAY CHARGES	56.54	56.54
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FULL ESTIMATED COST	86.49	256.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-8.25	-8.25

IN FILE 'CAPLUS' AT 11:43:57 ON 29 AUG 2006

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L7 ANSWER 11 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:454201 CAPLUS

DOCUMENT NUMBER: 135:220712

TITLE: Enhanced fungicidal activity of  
N-chlorotaurine in nasal secretionAUTHOR(S): Nagl, Markus; Lass-Flörl, Cornelia; Neher, Andreas;  
Gunkel, Andreas; Gottardi, WaldemarCORPORATE SOURCE: Institute of Hygiene and Social Medicine,  
Leopold-Franzens-University of Innsbruck, Innsbruck,  
A-6010, AustriaSOURCE: Journal of Antimicrobial Chemotherapy (2001  
, 47(6), 871-874

CODEN: JACHDX; ISSN: 0305-7453

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The antifungal activity of N-chlorotaurine (NCT), a long-lived oxidant produced by stimulated human leukocytes, was investigated. Incubation of *Aspergillus* spp., *Candida* spp., *Fusarium* spp., *Penicillium* spp. and *Alternaria* spp. in 1% NCT (55 mM) for 1-4 h produced a log10 reduction in cfu of between 1 and 4. In samples of nasal secretion, killing was significantly hastened (30 min), which may be explained by the formation of monochloramine by halogenation of ammonium, which was found at a concentration

of 1 mM in these samples. For these reasons, NCT is of interest as an agent for treatment of local inflammatory mycosis, e.g. eosinophilic fungal rhinosinusitis.

IT 51036-13-6, N-Chlorotaurine

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(enhanced fungicidal activity of N-chlorotaurine in nasal secretion)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

 $\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$ 

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:401649 CAPLUS

DOCUMENT NUMBER: 135:208038

TITLE: The influence of plasma on the disinfecting  
activity of the new antimicrobial agentAUTHOR(S): N-chlorotaurine sodium in comparison with chloramine T  
Gottardi, Waldemar; Hagleitner, Magdalena; Nagl,  
MarkusCORPORATE SOURCE: Institute for Hygiene und Social Medicine, University  
of Innsbruck, Innsbruck, AustriaSOURCE: Journal of Pharmacy and Pharmacology (2001),  
53(5), 689-697

CODEN: JPPMAB; ISSN: 0022-3573

PUBLISHER: Pharmaceutical Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The phenomenon of increasing bactericidal activity of N-chlorotaurine in the presence of Cl-consuming material was investigated both chemical-anal. and microbiol. by using plasma as substrate and chloramine T for comparison. Cl consumption, as assessed by iodometric titration, showed a biphasic time-course, with a very fast loss of oxidation capacity within 1 min (N-chlorotaurine: -9.3%, chloramine T: -16.8%), followed by a slow loss, so that activity could still be detected after 24 h (total loss -61.7% and -74.1%, resp.). Killing curves revealed that a plasma-induced increase in bactericidal activity, in spite of improved Cl consumption, did not occur against all strains and could be detected only at a certain degree of consumption. *Escherichia coli* and *Pseudomonas aeruginosa* were the most sensitive, *Streptococcus pyogenes* and *Proteus mirabilis* less so, and *Staphylococcus aureus* was not affected. With chloramine T, plasma caused no increase in bactericidal activity. The chemical basis of these Cl-consumption effects was limited to 4 reaction types: oxidation of thiols; Cl substitution of activated CH compds.; transhalogenation; and hydrolytic degradation of N-chloro- $\alpha$ -amino acids and -peptides emerging by transhalogenation. The initial fast loss of oxidation capacity could be attributed mainly to oxidation of thiols, while the subsequent slower decrease was caused by the other types of reaction. The increase in bactericidal activity, on the other hand, can be explained by transhalogenation, leading to the formation of more bactericidal N-chloro compds., by which the loss of N-chlorotaurine is overcompensated.

IT 51036-13-6, N-Chlorotaurine  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIC (Biological information)  
(plasma effect on the disinfecting activity of  
N-chlorotaurine in comparison with chloramine T)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 13 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:618660 CAPLUS

DOCUMENT NUMBER: 133:290708

TITLE: Bactericidal activity of micromolar N-chlorotaurine: evidence for its antimicrobial function in the human defense system

AUTHOR(S): Nagl, Markus; Hess, Michael W.; Pfaller, Kristian; Hengster, Paul; Gottardi, Waldemar

CORPORATE SOURCE: Institute of Hygiene and Social Medicine, Leopold-Franzens-University of Innsbruck, Innsbruck, A-6010, Austria

SOURCE: Antimicrobial Agents and Chemotherapy (2000), 44(9), 2507-2513

CODEN: AMACCQ; ISSN: 0066-4804

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-Chlorotaurine, the main representative of long-lived oxidants found in the supernatant of stimulated granulocytes, has been investigated systematically with regard to its antibacterial activity at different physiol. concns. for the first time. N-Chlorotaurine (12.5 to 50  $\mu$ M) demonstrated a bactericidal effect i.e., a 2 to 4 log<sub>10</sub> reduction in

viable counts, after incubation at 37 for 6 to 9 h at pH 7.0, which effect was significantly enhanced in an acidic milieu (at pH 5.0), with a 3 to 4 log<sub>10</sub> reduction after 2 to 3 h. Moreover, bacteria were attenuated after being incubated in N-chlorotaurine for a sublethal time, as demonstrated with the mouse peritonitis model. The supernatant of stimulated granulocytes exhibited similar activity. TEM revealed changes in the bacterial cell membrane and cytoplasmic disintegration with both reacting systems, even in the case of a mere attenuation. The results of this study suggest a significant bactericidal function of N-chlorotaurine and other chloramines during inflammation.

IT 51036-13-6, N-Chlorotaurine  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(bactericidal activity of micromolar N-chlorotaurine: evidence for its antimicrobial function in the human defense system)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE PE FORMAT

L7 ANSWER 14 ON 33 CAPLUS COPYRIGHT 2000 ACS ON JIN

ACCESSION NUMBER: 2000:544043 CAPLUS

DOCUMENT NUMBER: 134:141367

TITLE: Antimicrobial and cytotoxic activity of hypochlorous acid: interactions with taurine and nitrite

AUTHOR(S): Marcinkiewicz, J.; Chain, B.; Nowak, B.; Grabowska, A.; Bryniarski, K.; Baran, J.

CORPORATE SOURCE: Department of Immunology, Jagiellonian University Medical College, Krakow, 31-121, Pol.

SOURCE: Inflammation Research (2000), 49(6), 280-289  
CODEN: INREFB; ISSN: 1023-3830

PUBLISHER: Birkhaeuser Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Objective: Hypochlorous acid (HOCl), a major bactericidal product of neutrophil MPO - halide system reacts with taurine to form taurine chloramine (TauCl), a less toxic anti-inflammatory mediator. Recently, it has been reported that HOCl may also react with nitrite (NO<sub>2</sub>-), a major end-product of nitric oxide (NO) metabolism, to form very active oxidant, nitryl chloride (NO<sub>2</sub>Cl). The present study was conducted to elucidate the effect of nitrite on bactericidal and some immunoregulatory properties of HOCl and TauCl. Materials: TauCl was prepared from NaOCl and taurine. The reaction was carried out at pH 5.0 and pH 7.4, in the presence or absence of nitrite. All reactions were monitored by UV absorption spectra. Methods: Bactericidal activity of HOCl and TauCl in the presence of nitrite was tested by incubation of E. coli with the compds. and determined by the pour-plate method. To test the effect of the compds. on activity of inflammatory cells, murine peritoneal neutrophils (PMN) and macrophages were used. The cells were activated in vitro with either LPS, IFN-γ or zymosan and the production of following mediators was measured: reactive oxygen species using luminol-dependent chemiluminescence; nitric oxide by Griess reaction; TNF-α using capture ELISA. In addition, we tested the effect of HOCl and TauCl on activity of myeloperoxidase (MPO). Results:

At physiol. pH nitrite reacts with HOCl but not with TauCl. This reaction was abolished in the presence of taurine. Nitrite prevented HOCl-mediated bacterial killing, inhibition of MPO activity, cellular cytotoxicity and inhibition of TNF- $\alpha$  Production. Nitrite did not affect any activity of TauCl. Conclusion: We have shown that nitrite may react in vitro with HOCl but not with TauCl, to form new biol. active product(s). We did not confirm the hypothesis that a product of HOCl reaction with nitrite is more toxic than HOCl. To the contrary, we found that nitrite diminished bactericidal and immunoregulatory properties of HOCl. In vivo, nitrite will also compete with taurine for reaction with PMN-released HOCl. Nevertheless, due to high concentration of taurine in PMN cytosol, formation of TauCl will be a major regulatory mechanism of MPO-halide-system.

IT 51036-13-6, Taurine chloramine  
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)  
 (antimicrobial and cytotoxic activity of hypochlorous acid and interactions with taurine and nitrite)  
 RN 51036-13-6 CAPLUS  
 CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THIS FORMAT

L7 ANSWER 15 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:246164 CAPLUS

DOCUMENT NUMBER: 132:260249

TITLE: Tolerance of N-chlorotaurine, a new antimicrobial agent, in infectious conjunctivitis - a phase II pilot study

AUTHOR(S): Nagl, Markus; Teuchner, Barbara; Pottinger, Ernst; Ulmer, Hanno; Gottardi, Waldemar

CORPORATE SOURCE: Institute for Hygiene of the Leopold Franzens University of Innsbruck, University Hospital of Innsbruck, Austria

SOURCE: Ophthalmologica (2000), 214(2), 111-114  
 CODEN: OPHTAD; ISSN: 0030-3755

PUBLISHER: S. Karger AG

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-Chlorotaurine (NCT) is an endogenous microbicidal oxidant. This open pilot study (phase IIa) with 9 patients was done to gain first knowledge on the tolerance of NCT in infectious conjunctivitis. By application of 1% NCT 5 times a day, no adverse effects could be observed. All 6 subjects with bacterial conjunctivitis were cured within 3-5 days. Two subjects with epidemic keratoconjunctivitis were treated for 7-10 days and 1 subject with herpes simplex blepharitis for 3 days with no rapid improvement but probable mitigation of inflammation. Therefore, NCT seems to be useful in the treatment of infectious conjunctivitis, and further investigation on its therapeutic efficacy is suggested.

IT 51036-13-6, N-Chlorotaurine  
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (tolerability and effect of new antimicrobial N-Chlorotaurine in humans with infectious conjunctivitis)



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RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:408783 CAPLUS

DOCUMENT NUMBER: 131:179357

TITLE: The postantibiotic effect of N-chlorotaurine on Staphylococcus aureus. application in the mouse peritonitis model

AUTHOR(S): Nagl, Markus; Hengster, Paul; Semenitz, Erich; Gottardi, Waldemar

CORPORATE SOURCE: Institute for Hygiene, Leopold-Franzens-University of Innsbruck, Innsbruck, A-6010, Austria

SOURCE: Journal of Antimicrobial Chemotherapy (1999), 43(6), 805-809

CODEN: JACHDX; ISSN: 0305-7453

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This study was designed to investigate the delay of regrowth (postantibiotic effect) in the presence of N-chlorotaurine (NCT), an endogenous active N-chlorine compound, of Staphylococcus aureus, strain Smith diffuse. The low reactivity of NCT enabled clear temporal separation of the postantibiotic and killing effect to be defined. Delay of regrowth proved to be dependent both on concentration of NCT, and incubation time. The maximum delay was 3 h. Using the model of lethal staphylococcal peritonitis in mice, in-vivo delay of regrowth of bacteria pretreated with N-chlorotaurine could be demonstrated to correlate with survival. It is concluded that the postantibiotic effect of N-chlorotaurine could be an important factor on decreasing virulence of bacteria. This effect was observed after relatively short incubation times.

IT 51036-13-6, N-Chlorotaurine

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(postantibiotic effect of N-chlorotaurine on Staphylococcus aureus. application)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 17 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:1529 CAPLUS

DOCUMENT NUMBER: 130:150813

TITLE: Rapid killing of Mycobacterium terrae by N-chlorotaurine in the presence of ammonium is caused by the reaction product monochloramine

Roy P. Issac 10/825,288

29/08/2006

Roy P. Issac 10/825,288

AUTHOR(S): Nagl, Markus; Gottardi, Waldemar  
CORPORATE SOURCE: Institute for Hygiene, Leopold-Franzens University of  
Innsbruck, Innsbruck, A-6010, Austria  
SOURCE: Journal of Pharmacy and Pharmacology (1998),  
50(11), 1317-1320  
CODEN: JPPMAB; ISSN: 0022-3573  
PUBLISHER: Royal Pharmaceutical Society of Great Britain  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB We have studied the activity of the weak endogenous oxidant  
N-chlorotaurine against Mycobacterium terrae. The study revealed slow  
killing of more than 2 h duration by 1% (55 mM) N-chlorotaurine. In the  
presence of ammonium chloride, however, killing times decreased to a few  
minutes, even by 0.1% N-chlorotaurine. This phenomenon is explained by  
formation of the lipophilic and therefore more bactericidal monochloramine  
as a result of transhalogenation of ammonia by N-chlorotaurine.  
IT 51036-13-6, N-Chlorotaurine  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); RCT (Reactant); BIOL (Biological study); RACT  
(Reactant or reagent)  
(rapid killing of Mycobacterium terrae by chlorotaurine in the presence  
of ammonium is caused by the reaction product monochloramine)  
RN 51036-13-6 CAPLUS  
CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 18 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1998:703697 CAPLUS  
DOCUMENT NUMBER: 129:298001  
TITLE: Tolerance and bactericidal action of N-chlorotaurine  
in urinary tract infection by an omniresistant  
Pseudomonas aeruginosa  
AUTHOR(S): Nagl, Markus; Pfausler, Bettina; Schmutzhard, Erich;  
Fille, Manfred; Gottardi, Waldemar  
CORPORATE SOURCE: Inst. Hygiene, Leopold-Franzens-Univ., Innsbruck,  
A-6010, Austria  
SOURCE: Zentralblatt fuer Bakteriologie (1998),  
288(2), 217-223  
CODEN: ZEBAE8; ISSN: 0934-8840  
PUBLISHER: Gustav Fischer Verlag  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A case report is given on the N-chlorotaurine treatment of cystitis caused  
by P. aeruginosa inflammation of the upper urinary tract perpetuated by  
intravesical concrements. Repeated daily lavages of the urinary bladder  
(1%, 1 mo) were well tolerated. Despite killing of >10<sup>6</sup> cfu/mL within 10  
min in vitro and in vivo, the infection was not eradicated. The authors  
suggest that in localized infection treatment might be successful because  
of its sufficient bactericidal action.  
IT 51036-13-6, N-Chlorotaurine  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES  
(Uses)  
(tolerance and bactericidal action of N-chlorotaurine in urinary tract

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infection by an omniresistant *Pseudomonas aeruginosa*)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L7 ANSWER 19 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:689249 CAPLUS

DOCUMENT NUMBER: 129:270605

TITLE: Medicament based on singlet oxygen-producing agent

INVENTOR(S): Stief, Thomas W.

PATENT ASSIGNEE(S): Germany

SOURCE: Ger. Offen., 6 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19712565	A1	19981001	DE 1997-19712565	19970325 <--
PRIORITY APPLN. INFO.:			DE 1997-19712565	19970325

AB Substances which can give rise to singlet O and/or photodynamic treatment of diseases susceptible to singlet O or phototherapy, and can be used as anti-infective (especially antiviral) agents, immunostimulants, antithrombotics, and/or cytostatic agents. Viruses with a high concentration of cholesterol in the envelope, e.g. HIV, are especially susceptible to these agents. The agents may therefore be used for treating blood or blood products to inactivate viruses. Singlet O-generating substances can be stabilized by use as prodrugs or by addition of stabilizers such as taurine, carbonate salts, or mono- or oligosaccharides. Thus, N-chlorotaurine showed antithrombotic activity, as shown by dose-dependent prolongation of the thrombin, prothrombin, and activated partial thromboplastin times of citrated human plasma in vitro on addition of 2.5 or 3.3 mM N-chlorotaurine. N-chlorotaurine at 1 mM caused >1000-fold inactivation of HIV in whole blood within 15 min.

IT 51036-13-6, N-Chlorotaurine

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(medicament based on singlet oxygen-producing agent)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 20 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:561860 CAPLUS

DOCUMENT NUMBER: 129:314923

TITLE: Taurine chloramine inhibits the production of superoxide anion, IL-6 and IL-8 in activated human

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polymorphonuclear leukocytes

AUTHOR(S): Park, Eunhye; Alberti, James; Quinn, Michael R.; Schuller-Levis, Georgia

CORPORATE SOURCE: Departments of Immunology, NY State Institute Basic Research Developmental Disabilities, Staten Island, NY, 10314, USA

SOURCE: Advances in Experimental Medicine and Biology (1998), 442(Taurine 3), 177-182  
CODEN: AEMBAP; ISSN: 0065-2598

PUBLISHER: Plenum Publishing Corp.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Polymorphonuclear leukocytes (PMN) are the initial cells recruited to the site of inflammation where foreign invaders elicit an inflammation reaction. Activated PMN produce various oxygen and hydroxyl radicals which kill bacteria and fungi but may also induce indiscriminate cellular damage, e.g. by producing HOCl/OCl- by the halide-dependent myeloperoxidase. Taurine attenuates the damage caused by HOCl/OCl- by forming taurine chloramine. The effect of taurine chloramine on the production of various cytokines and superoxide anion by activated human PMN was investigated. Taurine chloramine down-regulates the production of superoxide anion, IL-6, and IL-8 by activated human PMN. The ability of taurine chloramine to modulate production of inflammatory modulators is not species specific and extends to human leukocytes.

IT 51036-13-6, Taurine chloramine  
RL: BAC (Biological activity or effector, except adverse); BCU (Biological study, unclassified); MFM (Metabolic formation); BIC (Biological study); FORM (Formation, nonpreparative)  
(taurine chloramine inhibits the production of superoxide anion, IL-6 and IL-8 in activated human polymorphonuclear leukocytes)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 21 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:414047 CAPLUS

DOCUMENT NUMBER: 129:130913

TITLE: Tolerance of N-chlorotaurine, an endogenous antimicrobial agent, in the rabbit and human eye. A phase I clinical study

AUTHOR(S): Nagl, Markus; Miller, Bruno; Daxecker, Franz; Ulmer, Hanno; Gottardi, Waldemar

CORPORATE SOURCE: Institute for Hygiene of the Leopold-Franzens-University of Innsbruck, Innsbruck, Austria

SOURCE: Journal of Ocular Pharmacology and Therapeutics (1998), 14(3), 283-290

CODEN: JOPTFU; ISSN: 1080-7683

PUBLISHER: Mary Ann Liebert, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-chlorotaurine (NCT), a compound produced by stimulated human leukocytes, has bactericidal, fungicidal, virucidal, and vermucidal efficacy. Irritation tolerance to the aqueous NCT solution was studied in the rabbit and human conjunctiva. In 6 rabbits treated with 1 and 3% NCT (1

drop 5-8 times daily for 9 days) no ocular and behavior changes were observed. In 2 volunteers, preliminary treatment with 2.8% NCT for 5 days caused a self-limited conjunctival vascular injection of one subject, while 1% NCT was well tolerated. Eight healthy volunteers participated in the phase I clin. study with 1% NCT. NCT was applied for 5 days and was well tolerated by all subjects except for minimal eye burning after the application. The use of the antimicrobial agent NCT in ophthalmol. is suggested.

IT 144557-26-6, Ethanesulfonic acid, 2-(chloroamino)-, monosodium salt

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(chlorotaurine tolerance in rabbit and human eye)

RN 144557-26-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)-, monosodium salt (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

● Na

REFERENCE COUNT: 17 THREE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD FORMAT

L7 ANSWER 22 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:313329 CAPLUS

DOCUMENT NUMBER: 129:12141

TITLE: High-performance liquid chromatographic analysis of amino acid- and peptide-derived chloramines

AUTHOR(S): Furness-Green, Suzanne M.; Inskeep, Tracy R.; Starke, Jennifer J.; Ping, Lu; Greenleaf-Schumann, Heather R.; Goyne, Thomas E.

CORPORATE SOURCE: Department of Chemistry, Valparaiso University, Valparaiso, IN, 46383, USA

SOURCE: Journal of Chromatographic Science (1998), 36(5), 227-236

CODEN: JCHSBZ; ISSN: 0021-9665

PUBLISHER: Preston Publications

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An isocratic reversed-phase HPLC method is reported for the anal. of amino acid- and peptide-derived chloramines (these are important intermediates in two very different processes: destruction of microbes by the neutrophil and disinfection of water with chlorine). Specifically, results are reported for the chloramines derived from the following amino acids and dipeptides: taurine, Ala, Gly, Ser, Thr, Phe, Val, AlaGly, GlyGly, PheGly, SerGly, and ValGly. Analyses were performed on a 250 + 4.6-mm C18 column using a buffered water-acetonitrile mixture as the mobile phase. For samples containing hydrophilic chloramines, an ion-pairing agent is added to the mobile phase. Two detection methods were used: direct UV detection of the chloramine at 254 nm and indirect UV detection of I<sup>3</sup>-at 350 nm following postcolumn reaction with iodide. Unexpectedly, the decomposition of amino acid-derived chloramines is found to greatly accelerate during chromatog. elution on a reversed-phase column.

IT 51036-13-6, Taurine chloramine 83152-69-6

RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST

29/08/2006

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(Analytical study); PROC (Process)

(high-performance liquid chromatog. anal. of amino acid- and peptide-derived chloramines)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

RN 83152-69-6 CAPLUS

CN Ethanesulfonic acid, 2-(dichloroamino)- (9CI) (CA INDEX NAME)

$\text{Cl}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 23 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:230582 CAPLUS

DOCUMENT NUMBER: 129:12317

TITLE: Activity of N-chlorotaurine against herpes simplex- and adenoviruses

AUTHOR(S): Nagl, M.; Larcher, C.; Waldemar  
JOURNAL SOURCE: Int. J. Hygiene, Leopold-Franke University of  
Innsbruck, Fritz-Pregl-Str. 3, Innsbruck, 6010,  
Austria

SOURCE: Antiviral Research (1998), 39(1), 25-30

CODEN: ARSRDR; ISSN: 0166-3542

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-chlorotaurine, an essential weak oxidant produced by stimulated human leukocytes, is known to have bactericidal, fungicidal and vermucidal properties. This study for the first time demonstrates its virucidal activity. By viral suspension tests at incubation times between 5 and 60 min, virus titers of both Herpes simplex virus type 1 and 2 were reduced about 1.3-2.9 log<sub>10</sub> and 2.8-4.2 log<sub>10</sub> by 0.1 and 1% (5.5 and 55 mM) N-chlorotaurine, resp. Virus titer reduction of adenovirus type 5 between 15 and 60 min was 0.5-2.0 and 0.6-4.0 log<sub>10</sub>, resp., by the same concns. of N-chlorotaurine. These findings support a contribution of N-chlorotaurine in destruction of pathogens during inflammatory reactions and also the possibility of its application as an antiviral agent in human medicine.

IT 51036-13-6, N-Chlorotaurine

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(activity of N-chlorotaurine against herpes simplex- and adenoviruses)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L7 ANSWER 24 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:287177 CAPLUS

DOCUMENT NUMBER: 124:312152

TITLE: Negative chemotaxis in *Cytophaga johnsonae*

AUTHOR(S): Liu, Zheng-Xian; Fridovich, Irwin

CORPORATE SOURCE: Dep. Biochem., Duke Univ. Medical Center, Durham, NC, 27710, USA

SOURCE: Canadian Journal of Microbiology (1996), 42(5), 515-518

CODEN: CJMIAZ; ISSN: 0008-4166

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chemotaxis, both pos. and neg., has been extensively studied in flagellated bacteria, such as *Escherichia coli* and *Salmonella typhimurium*, but not in gliding bacteria. The rapidly motile gliding bacterium *Cytophaga johnsonae* has been seen to be repelled by H<sub>2</sub>O<sub>2</sub>, OCl<sup>-</sup>, and N-chlorotaurine, as well as by low pH. Its response to H<sub>2</sub>O<sub>2</sub> was eliminated by catalase. Nalidixic acid at 200 µM, which inhibits the growth but not the motility of *C. johnsonae*, did not interfere with its neg. chemotactic response to H<sub>2</sub>O<sub>2</sub>, whereas sodium phosphate at 10 mM, which inhibits motility, did so. *Cytophaga johnsonae* was not repelled by taurine, n-octanol, phenol, L-valine, or high pH. Chemotaxis can be conveniently studied in gliding bacteria such as *C. johnsonae*.

IT 51036-13-6, N-Chlorotaurine

AC (Biological activity), effector, exptl. study; ECU (Biochem. study, unclassified); BIOL (Biological study) (neg. chemotaxis in *Cytophaga johnsonae*)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L7 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:197761 CAPLUS

DOCUMENT NUMBER: 124:252932

TITLE: Bacterial glutathione: a sacrificial defense against chlorine compounds

AUTHOR(S): Chesney, Jason A.; Eaton, John W.; Mahoney, John R., Jr.

CORPORATE SOURCE: Picower Institute, Manhasset, NY, 11030, USA

SOURCE: Journal of Bacteriology (1996), 178(7), 2131-35

CODEN: JOBAAY; ISSN: 0021-9193

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Aerobic organisms possess a number of often overlapping and well-characterized defenses against common oxidants such as superoxide and hydrogen peroxide. However, much less is known of mechanisms of defense against chlorine compds. Although chlorine-based oxidants may oxidize a number of cellular components, sulfhydryl groups are particularly reactive. The authors have, therefore, assessed the importance of intracellular glutathione in protection of *Escherichia coli* cells against hydrogen peroxide, hypochlorous acid, and chloramines. Employing a glutathione-deficient *E. coli* strain (JTG10) and an otherwise isogenic

glutathione-sufficient E. coli strain (AB1157), the authors find that glutathione-deficient organisms are approx. twice as sensitive to killing by both hydrogen peroxide and chlorine compds. However, the mode of protection by glutathione in these two cases appears to differ: exogenous glutathione added to glutathione-deficient E. coli in amts. equal to those which would be present in a similar suspension of the wild-type bacteria fully restored resistance of glutathione-deficient bacteria to chlorine-based oxidants but did not change resistance to hydrogen peroxide. Furthermore, in protection against chlorine compds., oxidized glutathione is almost as effective as reduced glutathione, implying that the tripeptide and/or oxidized thiol undergo further reactions with chlorine compds. Indeed, in vitro, 1 mol of reduced glutathione will react with .apprx.3.5 to 4.0 mol of hypochlorous acid. The authors conclude that glutathione defends E. coli cells against attack by chlorine compds. and hydrogen peroxide but, in the case of the halogen compds., does so nonenzymically and sacrificially.

IT 51036-13-6

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)  
(bacterial glutathione and defense against chlorine compds.)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

 $\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$ 

L7 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2000 ACS ON STN

ACCESSION NUMBER: 1993:189917 CAPLUS

DOCUMENT NUMBER: 118:189917

TITLE: Biotransformation of para-aminobenzoic acid and salicylic acid by PMN

AUTHOR(S): Sagone, Arthur L., Jr.; Husney, Rose Marie; Davis, W. Bruce

CORPORATE SOURCE: Dep. Intern. Med., Ohio State Univ., Columbus, OH, 43210, USA

SOURCE: Free Radical Biology &amp; Medicine (1993), 14(1), 27-35

CODEN: FRBMEH; ISSN: 0891-5849

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Para-aminobenzoic acid (PABA) is an essential cofactor for the production of folic acid in bacteria and has mild anti-inflammatory activity. Recently, it was reported that salicylic acid and benzoic acid are oxidized by stimulated granulocytic polymorphonuclear neutrophils (PMN). The oxidation of salicylate appeared to be mediated by a potent O metabolite generated during the respiratory burst which was dependent primarily on superoxide ( $\text{O}_2^-$ ) for its production. These background studies with the salicylate group of drugs suggested that PABA might be similarly metabolized by PMN. In these studies, PABA was metabolized by stimulated PMN. However, in contrast to the biochem. mechanism involved in the metabolism of salicylate, scavenger studies indicated that PABA was metabolized primarily by the myeloperoxidase pathway. These results may explain the mild anti-inflammatory actions of the drug and suggest that the degradation of PABA by PMN at an inflammatory site may limit the availability of PABA for bacterial growth.

IT 51036-13-6

RL: FORM (Formation, nonpreparative)

(formation of, by activated human neutrophil, salicylate inhibition of)

RN 51036-13-6 CAPLUS



29/08/2006

Roy P. Issac 10/825,288

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

L7 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:633436 CAPLUS

DOCUMENT NUMBER: 117:233436

TITLE: Preparation of N-chlorotaurine alkali metal salts as bactericides

INVENTOR(S): Gottardi, Waldemar

PATENT ASSIGNEE(S): Austria

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4041703	A1	19920702	DE 1990-4041703	19901224 <--
DE 4041703	C2	19931021		

PRIORITY APPLN. INFO.: DE 1990-4041703 19901224

OTHER SOURCE(S): M117:233436

AB  $\text{MSO}_3\text{CH}_2\text{CH}_2\text{NHCl}$  (I; M = alkali metal atom) were prepared as bactericides and disinfectants. Thus,  $\text{H}_2\text{NCH}_2\text{CH}_2\text{SO}_3\text{H}$  was stirred with 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>NCINa in EtOH to give I (M = Na) which had kill time of 0.75 min against Staphylococcus aureus at 1% concentration and pH 4.

IT 144557-26-6P 144557-27-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation of, as bactericide)

RN 144557-26-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)-, monosodium salt (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

● Na

RN 144557-27-7 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)-, monopotassium salt (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

● K

Roy P. Issac 10/825,288

L7 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:166247 CAPLUS

DOCUMENT NUMBER: 116:166247

TITLE: Use of zwitterionic compounds and their N-halo derivatives for stimulating myeloperoxidase activity and treating inflammation

INVENTOR(S): Bloomfield, Frederick Jacob

PATENT ASSIGNEE(S): Derma Systems Laboratories Ltd., Ire.

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 469813	A2	19920205	EP 1991-306903	19910729 <--
EP 469813	A3	19921119		
EP 469813	B1	19981230		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 9181332	A1	19920213	AU 1991-81332	19910725 <--
AU 641529	B2	19930923		
US 5248680	A	19930928	US 1991-736247	19910726 <--
CA 2048068	AA	19920131	CA 1991-2048068	19910729 <--
JP 05027655	A2	19930121	JP 1991-188644	19910729 <--
AT 175112	E	19930115	AT 1991-306903	19910729 <--
ES 2128309	T3	19990515	ES 1991-306903	19910729 <--

PRIORITY APPLN. INFO.: IE 1990-2741 A 19900730

AB Zwitterionic compds. (e.g. taurine, MES, HEPES, etc.) and their N-halo derivs. are used in the manufacture of a medicament for use as a stimulator of myeloperoxidase (MPO) activity and as an inflammation inhibitor. Intracerebroventricular injection of taurine (500µg) and i.p. injection of HEPES (500µg) produced a 54% and a 50% reduction in carrageenan-induced paw edema, resp.

IT 51036-13-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of and tablets containing, for inflammation inhibition)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L7 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:91608 CAPLUS

DOCUMENT NUMBER: 110:91608

TITLE: Determination of peroxidative halogenation in mixtures of chloride and bromide

AUTHOR(S): Ritter, Clare L.; Stead, Theresa M.; Malejka-Giganti, Danuta

CORPORATE SOURCE: Dep. Lab. Med. Pathol., Univ. Minnesota, Minneapolis, MN, USA

SOURCE: Analytical Biochemistry (1988), 174(1), 65-72

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

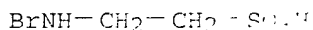
LANGUAGE: English

AB A method for the differentiation of chlorinated and brominated products from peroxidative oxidation of mixts. of the halides is presented. Chlorination or bromination of monochlorodimedone (MCD) by fungal chloroperoxidase (CPO) was measured by loss of MCD absorbance. Although the Vmax was similar for both halides [.apprx.0.08 mM (2 min)<sup>-1</sup>], the apparent Km for chlorination was 10 times greater than that for bromination (5.88 vs. 0.67 mM). Chlorination was also quantitated as I<sup>3</sup>- produced from N-chlorotaurine and I<sup>-</sup>. The Vmax [0.076 mM (2 min)<sup>-1</sup>] and apparent Km (6.31 mM) determined by this method agreed with those determined with MCD. Selective reduction by H<sub>2</sub>O<sub>2</sub> of the I<sup>-</sup> oxidizing potential of N-bromotaurine allowed determination of the brominated product from the difference between the amts. of halogenated MCD and N-chlorotaurine. The brominated product predominated at saturating and at physiol. halide levels. Hence, it is suggested that Br<sup>-</sup> plays a significant role in halogenation even though in vivo levels of Cl<sup>-</sup> are equal to or greater than 1000 times those of Br<sup>-</sup>.

IT 52316-57-1  
RL: FORM (Formation, nonpreparative)  
(formation of, by reaction of hypobromite with taurine)

RN 52316-57-1 CAPLUS

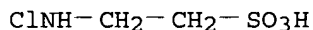
CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)



IT 51036-13-6, N-Chlorotaurine  
RL: FORM (Formation, nonpreparative)  
(formation of, by reaction of hypochlorite with taurine)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)



L7 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:434817 CAPLUS

DOCUMENT NUMBER: 107:34817

TITLE: Mutagenic activity of chloramines

AUTHOR(S): Thomas, Edwin L.; Jefferson, M. Margaret; Bennett, Jeffrey J.; Learn, Douglas B.

CORPORATE SOURCE: Dep. Biochem., St. Jude Child. Res. Hosp., Memphis, TN, 38101, USA

SOURCE: Mutation Research (1987), 188(1), 35-43  
CODEN: MUREAV; ISSN: 0027-5107

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mutagenesis by chloramines and HOCl was measured using the Salmonella typhimurium TA97a, TA100, and TA102 tester strains. Because chloramines and HOCl are bactericidal, react rapidly with cell components, and can destroy the histidine and biotin required for the mutagenesis assay, activity cannot be compared directly with that of less toxic or reactive agents. Nevertheless, chloramines were mutagenic when tested under appropriate conditions. TA100 was the most sensitive strain, and the most active mutagens were lipophilic dichloramines (RNCl<sub>2</sub>) including derivs. of histamine, ethanolamine, and putrescine. Lipophilic monochloramines

(RNHCl) such as histamine monochloramine and NH<sub>2</sub>Cl were less active. Hydrophilic chloramines such as taurine chloramines had low activity, and HOCl was inactive. The metabolic state of the bacteria was critical. Chloramines were mutagenic when added to bacteria with glucose at 37°, but killing predominated when chloramines were added at 4° or 25°, or at 37° without glucose. Production of chloramines and HOCl by leukocytes in vivo could contribute to the association of chronic inflammation and cancer as a result of: (1) the entry of membrane-permeable chloramines into normal cells followed by attack on intracellular components including DNA, and (2) the production of secondary mutagens such as compds. with carbonyl groups or C-Cl bonds. On the other hand, chlorination of water supplies is perhaps more likely to destroy than create mutagens, and chloramines from the environment are unlikely to penetrate the skin and mucous membranes.

IT 51036-13-6 83152-69-6

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)  
(mutagenicity of, in Ames test)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

RN 83152-69-6 CAPLUS

CN Ethanesulfonic acid, 2-(dichloroamino)- (9CI) (CA INDEX NAME)

Cl<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L7 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:136794 CAPLUS

DOCUMENT NUMBER: 106:136794

TITLE: Formation of hydrogen cyanide and its chlorination to cyanogen chloride by stimulated human neutrophils 2.  
Oxidation of thiocyanate as a source of HCN

AUTHOR(S): Stelmaszynska, Teresa

CORPORATE SOURCE: Inst. Med. Biochem., Copernicus Acad. Med., Krakow,  
31-034, Pol.

SOURCE: International Journal of Biochemistry (1986  
, 18(12), 1107-14

CODEN: IJBOBV; ISSN: 0020-711X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Leukocytes challenged by Staphylococcus epidermidis or stimulated by phorbol myristate acetate (PMA) produce cyanide from thiocyanate. The amount of H<sub>14</sub>CN formed depends on K<sub>14</sub>CN concentration and is enhanced by pretreatment of phagocytosed bacteria with penicillin or by adding amine-aurine to the medium of PMA-stimulated neutrophils. The reaction of taurine chloramine or chlorinated S. epidermidis (containing N-Cl groups) with thiocyanate results in HCN formation. At higher concentration of chloramine, cyanogen chloride is formed. Cyanide is chlorinated by PMA-stimulated neutrophils and this process is significantly enhanced by exogenous taurine and inhibited by 3-amino-1,2,4-triazole. It is conceivable that oxidation of thiocyanate to HCN and chlorination of HCN to cyanogen chloride is mediated by the chlorinating species (taurine chloramine) produced by stimulated neutrophils.

IT 51036-13-6

29/08/2006

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RL: BIOL (Biological study)  
(in hydrogen cyanide and cyanogen chloride formation by stimulated  
human neutrophil)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

L7 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:521552 CAPLUS

DOCUMENT NUMBER: 103:121552

TITLE: A possible origin of chemiluminescence in  
phagocytosing neutrophils. Reaction between  
chloramines and hydrogen peroxide

AUTHOR(S): Zgliczynski, Jan Maciej; Olszowska, Ewa; Olszowski,  
Slawomir; Stelmazynska, Teresa; Kwasnowska, Elzbieta

CORPORATE SOURCE: Inst. Biochem. Lek., Akad. Med., Krakow, 31034, Pol.

SOURCE: International Journal of Biochemistry (1985  
, 17(4), 515-19

CODEN: IJBOBV; ISSN: 0020-711X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A mixture of chloramines and  $\text{H}_2\text{O}_2$  emits light. The reaction between taurine  
monochloramine and  $\text{H}_2\text{O}_2$  is very rapid. The stoichiometry of the reaction  
is 1:1 and taurine is detected as one of the products. The chlorinated  
proteins and bacteria, containing N-Cl groups, when reacting with  
 $\text{H}_2\text{O}_2$ , are more effective in emitting light than low-mol. chloramines.  
Luminol enhances considerably the light yield of the chloramine- $\text{H}_2\text{O}_2$   
reaction. The chloramine- $\text{H}_2\text{O}_2$  reaction may account for light emitted by  
neutrophils during phagocytosis.

IT 51036-13-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with hydrogen peroxide, chemiluminescence in neutrophil  
phagocytosis in relation to)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

$\text{ClNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

L7 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1982:595021 CAPLUS

DOCUMENT NUMBER: 97:195021

TITLE: Myeloperoxidase-catalyzed incorporation of amines into  
proteins: role of hypochlorous acid and dichloramines

AUTHOR(S): Thomas, Edwin L.; Jefferson, M. Margaret; Grisham,  
Matthew B.

CORPORATE SOURCE: Cent. Health Sci., Univ. Tennessee, Memphis, TN,  
38101, USA

SOURCE: Biochemistry (1982), 21(24), 6299-308

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Myeloperoxidase-catalyzed oxidation of  $\text{Cl}^-$  to  $\text{HOCl}$  resulted in formation of  
mono- and dichloramine derivs. ( $\text{RNCHCl}$  and  $\text{RNC}_2$ ) of primary amines. The

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RNCl<sub>2</sub> derivs. could undergo a reaction that resulted in incorporation of the R moiety into proteins. The probable mechanism was attack of RNCl<sub>2</sub> or an intermediate formed in the decomposition of RNCl<sub>2</sub> on histidine, tyrosine, and cystine residues, and on lysine residues at high pH. Incorporation of radioactivity from labeled amines into stable, high-mol.-weight derivs. of proteins was measured by acid or acetone precipitation and by gel chromatog.

and

electrophoresis. Whereas formation of RNCl<sub>2</sub> was favored at low pH, the subsequent incorporation reaction was favored at high pH. Up to several h were required for the maximum amount of incorporation, which was <10% of the label in RNCl<sub>2</sub>. For the amines tested, incorporation was in the order: histamine > 1,2-diaminoethane > putrescine > taurine > lysine > glucosamine > leucine > methylamine. Initiation of the reaction required HOCl, and oxidized forms of Br-, I-, or SCN- did not substitute. Inhibitors of incorporation fell into 3 classes. (1) NH<sub>3</sub> or amines competed with the labeled amine for reaction with HOCl, so that larger amts. of HOCl were required. (2) Readily oxidized substances, such as thiols, diketo compds., or thioethers (methionine), reduced RNCl<sub>2</sub>. (3) Certain compds. competed with protein as acceptor for the incorporation reaction. The amount required to block incorporation into protein depended on protein concentration. Among these inhibitors were imidazole compds. (histidine), phenols (tyrosine), and disulfides (GSSG). Low yields of derivs. of histidine, tyrosine, and GSSG were detected by thin-layer chromatog. Acid-precipitable derivs. were obtained by reacting RNCl<sub>2</sub> with polyhistidine or polytyrosine, and to a lesser extent with polylysine at high pH, but not with other poly(amino acids). Precipitable derivs. were also obtained by incubating RNCl<sub>2</sub> with G-actin, which has a high content of substances with primary amino groups, which competed for incorporation. The results account for oxidative incorporation of amino acids into proteins in leukocytes and provide evidence that HOCl and N-Cl derivs. are formed in these cells. The characteristics of the incorporation reaction suggest that it would not contribute significantly to the antimicrobial activity of myeloperoxidase. Nevertheless, the reaction may provide a sensitive method for studying myeloperoxidase action in vivo.

IT 51036-13-6 83152-69-6

RL: BIOL (Biological study)

(in myeloperoxidase-catalyzed amine incorporation in proteins)

RN 51036-13-6 CAPLUS

CN Ethanesulfonic acid, 2-(chloroamino)- (9CI) (CA INDEX NAME)

ClNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

RN 83152-69-6 CAPLUS

CN Ethanesulfonic acid, 2-(dichloroamino)- (9CI) (CA INDEX NAME)

Cl<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

=> FIL HOME

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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374.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

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FILE 'HCAPLUS' ENTERED AT 11:36:55 ON 29 AUG 2006

FILE 'REGISTRY' ENTERED AT 11:37:01 ON 29 AUG 2006

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 13 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:38:06 ON 29 AUG 2006

L4 177 S L3

L5 156 S L4 AND 1800<=PY<=2004

L6 42 S L4 AND (DISINFECT? OR ANTIMICROB? OR ANTIBACT? OR BACTERIA OR

L7 33 S L6 AND L5

L8 1 S L7 AND (GLYCEROL OR ACNE OR CELLULOSE OR CETOMAKROGEL OR CETO

FILE 'HOME' ENTERED AT 11:44:31 ON 29 AUG 2006

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29/08/2006

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$\text{BrNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$

=> d his

(FILE 'HOME' ENTERED AT 18:08:48 ON 23 AUG 2006)

FILE 'REGISTRY' ENTERED AT 18:09:21 ON 23 AUG 2006

L1 STRUCTURE UPLOADED

L2 0 S L1 FAM SAM

L3 1 S L1 FAM FULL

FILE 'CAPLUS' ENTERED AT 18:10:52 ON 23 AUG 2006

L4 10 S L3



29/08/2006

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=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

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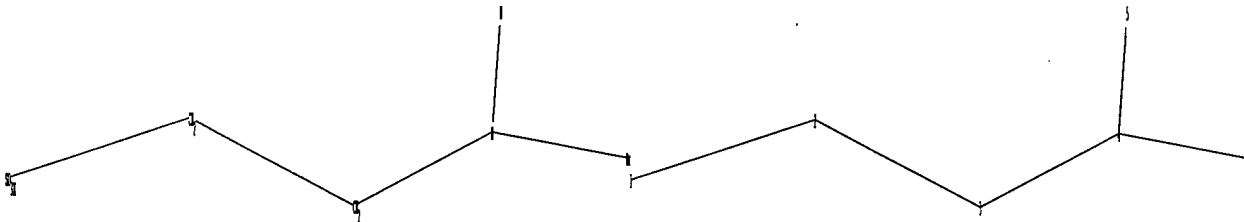
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Uploading C:\Program Files\Stnexp\Queries\288 bromo taurine.str



chain nodes :

1 2 3 4 5 6

chain bonds :

1-2 2-3 3-4 4-5 4-6

exact/norm bonds :

4-6

exact bonds :

1-2 2-3 3-4 4-5

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS

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29/08/2006

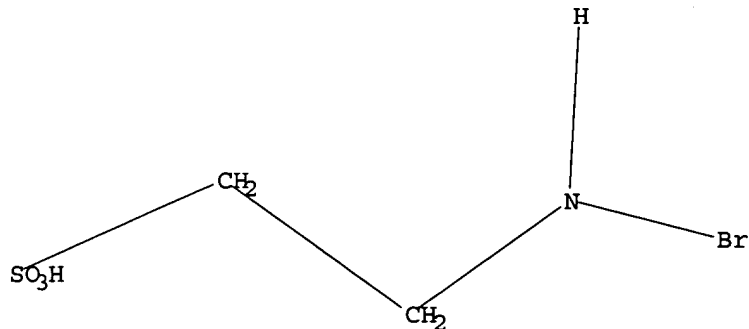
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 fam sam

SAMPLE SEARCH INITIATED 18:09:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA FAM SAM L1

=> s l1 fam full

FULL SEARCH INITIATED 18:10:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L3 1 SEA FAM FUL L1

=> d scan

L3 1 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Ethanesulfonic acid, 2-(bromoamino)- (9CI)

MF C2 H6 Br N O3 S

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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ALL ANSWERS HAVE BEEN SCANNED

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

66.57

66.78

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L4 10 L3

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4 IS NOT VALID HERE

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=> d ibib abs hitstr 1-4

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:481846 CAPLUS

DOCUMENT NUMBER: 143:166264

TITLE: Is there a role of taurine bromamine in inflammation?

Interactive effects with nitrite and hydrogen peroxide

AUTHOR(S): Marcinkiewicz, J.; Mak, M.; Bobek, M.; Biedron, R.;

Bialecka, A.; Koprowski, M.; Kontny, E.; Maslinski, W.

CORPORATE SOURCE: Department of Immunology, Jagiellonian University

Medical College, Krakow, 31-121, Pol.

SOURCE: Inflammation Research (2005), 54(1), 42-49

CODEN: INREFB; ISSN: 1023-3830

PUBLISHER: Birkhaeuser Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The myeloperoxidase system of neutrophils generates chlorinating and

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brominating oxidants in vivo. The major haloamines of the system are Tau chloramine (TauCl) and Tau bromamine (TauBr). It was demonstrated in vitro that TauCl exerts both anti-inflammatory and anti-bacterial properties. Much less is known about TauBr. The present study was conducted to compare bactericidal and immunoregulatory capacity of TauBr with that of the major chlorinating oxidants: HOCl and TauCl. Moreover, the effect of nitrites and H<sub>2</sub>O<sub>2</sub> on TauBr activity was investigated. TauBr was prepared by reaction of HOBr with Tau. The reaction was monitored by UV absorption spectra. Bactericidal activity of TauBr, TauCl, and HOCl was tested by incubation of *E. coli* with the compds. and determined by the pour-plate method. To test the anti-inflammatory activity the compds. were incubated with LPS-and IFN- $\gamma$  stimulated murine peritoneal macrophages. The production of following mediators was measured: nitrites by Griess reaction; TNF- $\alpha$ , IL-6, IL-10, IL-12p40 using capture ELISA. In some expts. the compds. were incubated with either nitrites or H<sub>2</sub>O<sub>2</sub>. In the authors' exptl. set-up TauBr and HOCl exerted strong bactericidal effects on *E. coli* (MBC = 110  $\mu$ M and 8  $\mu$ M, resp.), while TauCl (< 1000  $\mu$ M) did not kill test bacteria. However, both, TauBr and TauCl, at noncytotoxic concns. (< 300  $\mu$ M) inhibited the cytokine and nitric oxide production by macrophages. H<sub>2</sub>O<sub>2</sub> completely abolished the biol. activities of TauBr but not those of TauCl. Nitrites did not affect any activity of TauBr or TauCl while they diminished the HOCl- mediated bacterial killing. TauBr, despite very low concentration of Br- in body fluids,

may support TauCl and HOCl in the regulation of inflammatory response and in killing of bacteria by neutrophils. However, TauBr activity in vivo will depend on the presence of H<sub>2</sub>O<sub>2</sub> and possible other mediators of inflammation which can compete with target mols. for TauBr.

IT 52316-57-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(of taurine bromamine in inflammation interactive effects with nitrite and hydrogen peroxide)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:905635 CAPLUS

DOCUMENT NUMBER: 141:374694

TITLE: Method using taurine bromamine for inhibiting pathogenic bacteria and fungi growth, and microbicidal composition

INVENTOR(S): Marcinkiewicz, Janusz; Kasproicz, Andrzej

PATENT ASSIGNEE(S): Pol.

SOURCE: U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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29/08/2006

Roy P. Issac 10/825,288

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US 2004214891      A1      20041028      US 2004-825288      20040416
WO 2004093853      A2      20041104      WO 2004-PL27        20040420
WO 2004093853      A3      20060330
W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
    CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
    GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
    LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
    NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
    TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW:  BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
    BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
    ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
    SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
    TD, TG
EP 1663195      A2      20060607      EP 2004-728482      20040420
R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
    IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRIORITY APPLN. INFO.:      PL 2003-359792      A 20030422
                                PL 2004-367052      A 20040407
                                WO 2004-PL27      W 20040420
AB  In a method for inhibiting pathogenic bacteria and fungi growth, bacteria
    and fungi are treated with an effective quantity of taurine bromamine,.
    The effective quantity of taurine bromamine has concns. of 10-100 weight%.
    The microbicidal composition, of the invention contains taurine bromamine in
    concns. of 10-100 weight%.
IT  52316-57-1
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
        (Biological study); USES (Uses)
        (taurine bromamine for inhibiting pathogenic bacteria and fungi growth,
        and microbicidal composition)
RN  52316-57-1  CAPLUS
CN  Ethanesulfonic acid, 2-(bromoamino)- (9CI)  (CA INDEX NAME)

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BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

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L4  ANSWER 3 OF 10  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:      2001:675286  CAPLUS
DOCUMENT NUMBER:      136:65950
TITLE:      Oxidation of NADH by Chloramines and Chloramides and
            Its Activation by Iodide and by Tertiary Amines
AUTHOR(S):      Pruetz, Walter A.; Kissner, Reinhard; Koppenol, Willem
                H.
CORPORATE SOURCE:      Institut fuer Molekulare Medizin und Zellforschung,
                Universitaet Freiburg, Sektion Biophysik, Freiburg,
                D-79104, Germany
SOURCE:      Archives of Biochemistry and Biophysics (2001),
                393(2), 297-307
                CODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER:      Academic Press
DOCUMENT TYPE:      Journal
LANGUAGE:      English
AB  Irreversible oxidation of reduced nicotinamide nucleotides by
    neutrophil-derived halogen oxidants (HOCl, chloramines, HOBr, etc.) is
    likely to be a highly lethal process, because of the essential role of
    NAD(P)H in important cell functions such as mitochondrial electron
    transport, and control of the cellular thiol redox state by

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Roy P. Issac 10/825,288

NADPH-dependent glutathione reductase. Chloramines (chloramine-T,  $\text{NH}_2\text{Cl}$ , etc.) and N-chloramides (N-chlorinated cyclopeptides) react with NADH to generate the same products as  $\text{HOCl}$ , i.e., pyridine chlorohydrins, as judged from characteristic changes in the NADH absorption spectrum. Compared with the fast oxidation of NADH by  $\text{HOCl}$ ,  $k \approx 3 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$  at pH 7.2, the oxidation by chloramines is about five orders of magnitude slower; that by chloramides is about four orders of magnitude slower. Apparent rate consts. for oxidation of NADH by chloramines increase with increasing proton or buffer concentration, consistent with general acid catalysis, but oxidation by chloramides proceeds with pH-independent kinetics. In presence of iodide the oxidation of NADH by chloramines or chloramides is faster by at least two orders of magnitude; this is due to reaction of iodide with the N-halogen to give  $\text{HOI}/\text{I}_2$ , the most reactive and selective oxidant for NADH among  $\text{HOX}$  species. Quinuclidine derivs. (QN) like 3-chloroquinuclidine and quinine are capable of catalyzing the irreversible degradation of NADH by  $\text{HOCl}$  and by chloramines;  $\text{QN} + \text{Cl}$ , the chain carrier of the catalytic cycle, is even more reactive toward NADH than  $\text{HOCl}/\text{ClO}^-$  at physiol. pH. Oxidation of NADH by  $\text{NH}_2\text{Br}$  proceeds by fast, but complex, biphasic kinetics. A compilation of rate consts. for interactions of reactive halogen species with various substrates is presented and the concept of selective reactivity of N-halogens is discussed. (c) 2001 Academic Press.

IT 52316-57-1

RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)  
(oxidation of NADH by chloramines and chloramides and its activation by iodide and by tertiary amines)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

 $\text{BrNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$ 

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:216282 CAPLUS

DOCUMENT NUMBER: 135:4102

TITLE: Production of brominating intermediates by myeloperoxidase. A transhalogenation pathway for generating mutagenic nucleobases during inflammation  
AUTHOR(S): Henderson, Jeffrey P.; Byun, Jaeman; Williams, Michelle V.; Mueller, Dianne M.; McCormick, Michael L.; Heinecke, Jay W.

CORPORATE SOURCE: Department of Medicine, Washington University School of Medicine, St. Louis, MO, 63110, USA

SOURCE: Journal of Biological Chemistry (2001), 276(11), 7867-7875

CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The existence of interhalogen compds. was proposed more than a century ago, but no biol. roles have been attributed to these highly oxidizing intermediates. In this study, whether the peroxidases of white blood cells can generate the interhalogen gas bromine chloride ( $\text{BrCl}$ ) was determined. Myeloperoxidase, the heme enzyme secreted by activated neutrophils and

monocytes, used H<sub>2</sub>O<sub>2</sub> and Cl<sup>-</sup> to produce HOCl, a chlorinating intermediate. In contrast, eosinophil peroxidase preferentially converted Br<sup>-</sup> to HOBr. Remarkably, both myeloperoxidase and eosinophil peroxidase were able to brominate deoxycytidine, a nucleoside, and uracil, a nucleobase, at plasma concns. of Br<sup>-</sup> (100 µM) and Cl<sup>-</sup> (100 mM). The two enzymes used different reaction pathways, however. When HOCl brominated deoxycytidine, the reaction required Br<sup>-</sup> and was inhibited by taurine. In contrast, bromination by HOBr was independent of Br<sup>-</sup> and unaffected by taurine. Moreover, taurine inhibited 5-bromodeoxycytidine production by the myeloperoxidase-H<sub>2</sub>O<sub>2</sub>-Cl<sup>-</sup>-Br<sup>-</sup> system but not by the eosinophil peroxidase-H<sub>2</sub>O<sub>2</sub>-Cl<sup>-</sup>-Br<sup>-</sup> system, indicating that bromination by myeloperoxidase involves the initial production of HOCl. Both HOCl-Br<sup>-</sup> and the myeloperoxidase-H<sub>2</sub>O<sub>2</sub>-Cl<sup>-</sup>-Br<sup>-</sup> system generated a gas that converted cyclohexene into 1-bromo-2-chlorocyclohexane, implicating BrCl in the reaction. Moreover, human neutrophils used myeloperoxidase, H<sub>2</sub>O<sub>2</sub>, and Br<sup>-</sup> to brominate deoxycytidine by a taurine-sensitive pathway, suggesting that transhalogenation reactions may be physiol. relevant. 5-Bromouracil incorporated into nuclear DNA is a well-known mutagen. Perhaps transhalogenation reactions initiated by phagocytes provide one pathway for mutagenesis and cytotoxicity at sites of inflammation.

IT 52316-57-1

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(production of brominating intermediates by human neutrophil myeloperoxidase as a transhalogenation pathway for generating mutagenic nucleobases during inflammation)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

 $\text{BrNH}-\text{CH}_2-\text{CH}_2-\text{SO}_3\text{H}$ 

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:372246 CAPLUS

DOCUMENT NUMBER: 122:208432

TITLE: Oxidation of bromide by the human leukocyte enzymes myeloperoxidase and eosinophil peroxidase. Formation of bromamines

AUTHOR(S): Thomas, Edwin L.; Bozeman, Paula M.; Jefferson, M. Margaret; King, Charles C.

CORPORATE SOURCE: Dental Research Center, University of Tennessee, Memphis, TN, 38105, USA

SOURCE: Journal of Biological Chemistry (1995), 270(7), 2906-13

CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Myeloperoxidase and eosinophil peroxidase catalyzed the oxidation of Br<sup>-</sup> by H<sub>2</sub>O<sub>2</sub> and produced a brominating agent that reacted with amine compds. to form bromoamines, which are long-lived oxidants containing covalent N-Br

bonds. The results were consistent with oxidation of Br<sup>-</sup> to an equilibrium mixture

of HOBr and OBr<sup>-</sup>. Up to 1 mol of bromamine was produced per mol of H<sub>2</sub>O<sub>2</sub>, indicating that bromamine formation prevented the reduction of HOBr/OBr<sup>-</sup> by H<sub>2</sub>O<sub>2</sub> and the loss of oxidizing and brominating activity. Bromamines differed from HOBr/OBr<sup>-</sup> in that bromamines reacted slowly with H<sub>2</sub>O<sub>2</sub>, were not reduced by DMSO, and had absorption spectra similar to those of chloramines, but shifted 36 nm toward higher wavelengths. Mono- and di-Br derivs. (RNHBr and RNHBr<sub>2</sub>) of the β-amino acid, taurine, were relatively stable with half-lives of 70 and 16 h at pH 7, 37°. The monobromamine was obtained with a 200-fold excess of amine over the amount of HOBr/OBr<sup>-</sup> and the dibromoamine at a 2:1 ratio of HOBr/OBr<sup>-</sup> to the amine. In the presence of physiol. levels of both Br<sup>-</sup> (0.1 mM) and Cl<sup>-</sup> (0.1 M), myeloperoxidase and eosinophil peroxidase produced mixts. of bromamines and chloramines containing 6 and 88% bromamine, resp. In contrast, only the monochloramine derivative (RNHCl) was formed when a mixture of HOCl and OCl<sup>-</sup> was added to solns. containing Br<sup>-</sup> and excess amine. The rapid formation of the chloramine prevented the oxidation of Br<sup>-</sup> by HOCl/OCl<sup>-</sup>, and the chloramine did not react with Br<sup>-</sup> within 1 h at 37°. The results indicated that when enzyme-catalyzed Br<sup>-</sup> or Cl<sup>-</sup> oxidation took place in the presence of an amine compound at 10 mM or higher, bromamines were not produced in secondary reactions such as the oxidation of bromide by HOCl/OCl<sup>-</sup> and the exchange of Br<sup>-</sup> with Cl atoms of chloramines. Therefore, the amount of bromamine produced by myeloperoxidase or eosinophil peroxidase was equal to the amount of Br<sup>-</sup> oxidized by the enzyme. Br<sup>-</sup> was preferred over Cl<sup>-</sup> as the substrate for both enzymes.

IT 52316-57-1P

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(oxidation of bromide by human myeloperoxidase and eosinophil peroxidase and formation of bromamines)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:511333 CAPLUS

DOCUMENT NUMBER: 113:111333

TITLE: Characterization of vanadium bromoperoxidase from Macrocystis and Fucus: reactivity of vanadium bromoperoxidase toward acyl and alkyl peroxides and bromination of amines

AUTHOR(S): Soedjak, Helena S.; Butler, Alison

CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, 93106, USA

SOURCE: Biochemistry (1990), 29(34), 7974-81

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Vanadium bromoperoxidase (V-BrPO) was isolated and purified from the marine brown algae, *F. distichus* and *M. pyrifera*. V-BrPO catalyzed the oxidation of Br<sup>-</sup> by H<sub>2</sub>O<sub>2</sub> resulting in the bromination of certain organic acceptors or the formation of O<sub>2</sub>. V-BrPO from *F. distichus* and *M. pyrifera* had subunit mol. wts. of 65 and 75 kDa, resp., and specific activities of 1580 (pH 6.5) and 1730 units mg (pH 6), resp. for the bromination of monochlorodimedone. As isolated, the enzymes contained a



substoichiometric V/subunit ratio; the V content and specific activity was increased by the addition of vanadate. V-BrPO (*F. distichus*, *M. pyrifera*, and *Ascomyllum nodosum*) also catalyzed the oxidation of Br<sup>-</sup> using peracetic acid. In the absence of an organic acceptor, a mixture of oxidized Br species (e.g., hypobromous acid, Br<sub>2</sub>, and tribromide) was formed. Bromamine derivs. were formed from the corresponding amines, whereas 5-bromocytosine was formed from cytosine. In all cases, the rate of the V-BrPO-catalyzed reaction was much faster than that of the uncatalyzed oxidation of Br<sup>-</sup> by peracetic acid, at pH 8.5, 1 mM Br<sup>-</sup>, and 2 mM peracetic acid. In contrast to H<sub>2</sub>O<sub>2</sub>, V-BrPO did not catalyze the formation of O<sub>2</sub> from peracetic acid in either the presence or absence of Br<sup>-</sup>. V-BrPO also used phenylperacetic acid, m-chloroperoxybenzoic acid, and p-nitroperoxybenzoic acid to catalyze the oxidation of Br<sup>-</sup>; O<sub>2</sub> was not formed with these peracids. V-BrPO did not catalyze Br<sup>-</sup> oxidation nor O<sub>2</sub> formation with the alkyl peroxides, Et hydroperoxide, tert-Bu hydroperoxide, and cuminyl hydroperoxide.

IT 52316-57-1

RL: FORM (Formation, nonpreparative)

(formation of, by bromoperoxidase of marine algae)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:548599 CAPLUS

DOCUMENT NUMBER: 111:148599

TITLE: Oxidations of the carcinogen N-hydroxy-N-(2-fluorenyl)acetamide by enzymically or chemically generated oxidants of chloride and bromide

AUTHOR(S): Ritter, Clare L.; Malejka-Giganti, Danuta

CORPORATE SOURCE: Dep. Lab. Med. Pathol., Univ. Minnesota, Minneapolis, MN, 55447, USA

SOURCE: Chemical Research in Toxicology (1989), 2(5), 325-33  
CODEN: CRTOC; ISSN: 0893-228X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The oxidns. of N-hydroxy-N-(2-fluorenyl)acetamide (N-OH-2-FAA) via 1-electron (1e<sup>-</sup>) oxidation to equimolar 2-nitrosofluorene (2-NOR) and N-acetoxy-2-FAA and via oxidative cleavage to 2-NOF by the oxidants Cl<sup>-</sup> and/or Br<sup>-</sup> generated chemical and by myeloperoxidase (MPO)/H<sub>2</sub>O<sub>2</sub> were investigated. 2-NOF was determined spectrophotometrically in the reaction mixts. and by HPLC of their exts.; N-acetoxy-2-FAA was determined by HPLC. In the presence of individual or mixed halides at their physiol. concns. [0.1M Cl<sup>-</sup> and/or 0.1 mM Br<sup>-</sup>] and pH ~6, MPO-H<sub>2</sub>O<sub>2</sub>-catalyzed oxidation of N-OH-2-FAA to 2-NOF via oxidative cleavage was much greater than 1e<sup>-</sup> oxidation. At the resp. pH optima, oxidation was much more rapid with Br<sup>-</sup> and Br<sup>-</sup> + Cl<sup>-</sup> than with Cl<sup>-</sup>. HOBr or HOCl + Br<sup>-</sup> oxidized N-OH-2-FAA more rapidly than HOCl, also chiefly via oxidative cleavage. This suggested that, in the presence of MPO/H<sub>2</sub>O<sub>2</sub> + Cl<sup>-</sup> + Br<sup>-</sup>, oxidation was due to HOBr from HOCl oxidation of Br<sup>-</sup> and/or oxidation of Br<sup>-</sup> by MPO/H<sub>2</sub>O<sub>2</sub>. In the presence of taurine

(1 or 10 mM), a scavenger of hypohalous acids, MPO-H<sub>2</sub>O<sub>2</sub> catalysis of oxidative cleavage was unaffected with Br<sup>-</sup>, prevented with Cl<sup>-</sup> and partially prevented with Cl<sup>-</sup> + Br<sup>-</sup>. These were linked to N-halotaurine formation since N-bromotaurine, but not N-chlorotaurine, oxidized N-OH-2-FAA chiefly to 2-NOF. With time N-chlorotaurine and N-bromotaurine appeared to

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undergo a pH-dependent halide exchange with B and Cl, resp. Apparently, oxidants of Br may play a role in vivo in the activation of carcinogens.

IT 52316-57-1

RL: BIOL (Biological study)  
(hydroxy(fluorenyl)acetamide oxidation by)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:91608 CAPLUS

DOCUMENT NUMBER: 110:91608

TITLE: Determination of peroxidative halogenation in mixtures of chloride and bromide

AUTHOR(S): Ritter, Clare L.; Stead, Theresa M.; Malejka-Giganti, Danuta

CORPORATE SOURCE: Dep. Lab. Med. Pathol., Univ. Minnesota, Minneapolis, MN, USA

SOURCE: Analytical Biochemistry (1988), 174(1), 65-72

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method for the differentiation of chlorinated and brominated products from peroxidative oxidation of mixts. of the halides is presented. Chlorination or bromination of monochlorodimedone (MCD) by fungal chloroperoxidase (CPO) was measured by loss of MCD absorbance. Although the V<sub>max</sub> was similar for both halides [apprx.0.08 mM (2 min)<sup>-1</sup>], the apparent K<sub>m</sub> for chlorination was 10 times greater than that for bromination (5.88 vs. 0.67 mM). Chlorination was also quantitated as I<sup>3</sup>- produced from N-chlorotaurine and I<sup>-</sup>. The V<sub>max</sub> [0.076 mM (2 min)<sup>-1</sup>] and apparent K<sub>m</sub> (6.31 mM) determined by this method agreed with those determined

with

MCD. Selective reduction by H<sub>2</sub>O<sub>2</sub> of the I<sup>-</sup> oxidizing potential of N-bromotaurine allowed determination of the brominated product from the

difference

between the amts. of halogenated MCD and N-chlorotaurine. The brominated product predominated at saturating and at physiol. halide levels. Hence, it is suggested that Br<sup>-</sup> plays a significant role in halogenation even though in vivo levels of Cl<sup>-</sup> are equal to or greater than 1000 times those of Br<sup>-</sup>.

IT 52316-57-1

RL: FORM (Formation, nonpreparative)  
(formation of, by reaction of hypobromite with taurine)

RN 52316-57-1 CAPLUS

CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:568290 CAPLUS

DOCUMENT NUMBER: 107:168290

TITLE: Killing of schistosomula by taurine chloramine and taurine bromamine

AUTHOR(S): Yazdanbakhsh, Maria; Eckmann, Carel M.; Roos, Dirk

Roy P. Issac 10/825,288

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Roy P. Issac 10/825,288

CORPORATE SOURCE: Cent. Lab., Netherlands Red Cross Blood Transfus.  
Serv., Amsterdam, Neth.  
SOURCE: American Journal of Tropical Medicine and Hygiene  
(1987), 37(1), 106-10  
CODEN: AJTHAB; ISSN: 0002-9637  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Both taurine chloramine and taurine bromamine at 100  $\mu$ M are able to  
kill the schistosomula of *Schistosoma mansoni*. The production of these 2  
comps. may be part of the mechanism by which eosinophils kill *S. mansoni*  
in vivo.  
IT 52316-57-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of and *Schistosoma mansoni* killing by)  
RN 52316-57-1 CAPLUS  
CN Ethanesulfonic acid, 2-(bromoamino)- (9CI) (CA INDEX NAME)

BrNH-CH<sub>2</sub>-CH<sub>2</sub>-SO<sub>3</sub>H

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1974:112519 CAPLUS  
DOCUMENT NUMBER: 80:112519  
TITLE: Dental compositions  
INVENTOR(S): Vit, Jaroslav  
PATENT ASSIGNEE(S): National Patent Development Corp.  
SOURCE: Ger. Offen., 22 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2329752	A1	19740131	DE 1973-2329752	19730612
US 3932605	A	19760113	US 1972-301163	19721026
AU 7356652	A1	19741212	AU 1973-56652	19730607
CA 995586	A1	19760824	CA 1973-173632	19730608
FR 2187289	A1	19740118	FR 1973-21264	19730612
JP 49048848	A2	19740511	JP 1973-66279	19730612
JP 60018642	B4	19850511		
US 3998945	A	19761221	US 1975-589683	19750624
CA 1036846	A2	19780822	CA 1978-295000	19780116
JP 55089218	A2	19800705	JP 1979-56837	19790507
JP 60019889	B4	19850518		

PRIORITY APPLN. INFO.:  
GB 1972-27443 A 19720612  
GB 1972-30611 A 19720629  
GB 1972-39588 A 19720824  
GB 1972-39589 A 19720824  
US 1972-301141 A 19721026  
US 1972-301163 A 19721026  
CA 1973-173630 A3 19730608

AB Solns. for removal of plaque and calculus from teeth and caries-preventing  
tooth pastes and mouthwashes contained a halogenated amine, e.g.  
N-halogenated glycine, sulfamic acid, taurine, or eDTA, optionally formed  
from the amine and hypohalite, e.g. NaOCl. Thus, a tooth paste contained  
NaCl 44, NaHCO<sub>3</sub> 24, CaCO<sub>3</sub> 21.5, Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> 5.0, KCl 3.5, MgSO<sub>4</sub> 1.75, and

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	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

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=> e taurine bromamine

E1	1	TAURINDICUS/BI
E2	17095	TAURINE/BI
E3	0 -->	TAURINE BROMAMINE/BI
E4	3	TAURINE16/BI
E5	1	TAURINE4/BI
E6	4	TAURINEAMIDE/BI
E7	2	TAURINEBETAINE/BI
E8	1	TAURINECARBODITHIOATE/BI
E9	2	TAURINECHLORAMINE/BI
E10	1	TAURINECHLORETHYLNITROSUREA/BI
E11	1	TAURINEDIACETIC/BI
E12	1	TAURINEDITHIOCARBOXYLATE/BI

=> FIL BIOSCIENCE

FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED  
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	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.06	5.27

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=> e taurine bromamine

E1	28	TAURINDICUS/BI
E2	91568	TAURINE/BI
E3	0	--> TAURINE BROMAMINE/BI
E4	1	TAURINE+LEUPEPTINCEPTOR/BI
E5	1	TAURINE1/BI
E6	8	TAURINE16/BI
E7	1	TAURINE22/BI
E8	2	TAURINE4/BI
E9	2	TAURINEALPHA/BI
E10	41	TAURINEAMIDE/BI
E11	2	TAURINEAMINE/BI
E12	1	TAURINEAND/BI

=> FIL CHEMISTRY PHARMACOLOGY

FILE 'ENCOMPLIT2' ACCESS NOT AUTHORIZED

FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
91.21	96.48

FULL ESTIMATED COST

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=> e taurine bromamine

E1	28	TAURINDICUS/BI
E2	93699	TAURINE/BI
E3	0	--> TAURINE BROMAMINE/BI
E4	1	TAURINE+LEUPEPTINCEPTOR/BI
E5	1	TAURINE1/BI
E6	1	TAURINE15/BI
E7	9	TAURINE16/BI
E8	1	TAURINE22/BI
E9	4	TAURINE4/BI
E10	1	TAURINEALKYLAMIDE/BI
E11	2	TAURINEALPHA/BI

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=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

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=> e bromo taurine

E1	1	BROMNYKH/BI
E2	145199	BROMO/BI
E3	0 -->	BROMO TAURINE/BI
E4	1	BROMO0/BI
E5	15	BROMO1/BI
E6	1	BROMO10/BI
E7	1	BROMO11/BI
E8	2	BROMO17/BI
E9	33	BROMO2/BI
E10	13	BROMO3/BI
E11	13	BROMO4/BI
E12	5	BROMO5/BI

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

2.53

2.74

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=> d his

(FILE 'HOME' ENTERED AT 15:27:07 ON 28 AUG 2006)

FILE 'BIOSIS' ENTERED AT 15:29:06 ON 28 AUG 2006

E "(TAURINE BROMAMINE) OR (BROMOAMINO ETHANESULFONIC)"/CN 25

E " (BROMOAMINO ETHANESULFONIC)"/CN 25

E " (BROMOAMINO ETHANESULFONIC ACID)"/CN 25

E "TAURINE CHLORAMINE"/CN 25

L1 64 S E3

FILE 'REGISTRY' ENTERED AT 15:36:06 ON 28 AUG 2006

L2 1 S 51036-13-6/RN

SET NOTICE 1 DISPLAY

SET NOTICE LOGIN DISPLAY

SET NOTICE 1 DISPLAY

SET NOTICE LOGIN DISPLAY

FILE 'HCAPLUS' ENTERED AT 15:37:44 ON 28 AUG 2006

E "51036-13-6"/BI,RN 25

L3 162 S E3

L4 162 S E3 OR E5 OR E6

L5 84 S L4 AND (ACNE OR ANTI? OR BACTER? OR FUNG? OR DISINFECT?)

L6 0 S L5 AND (ACNE)

L7 0 S L5 AND (DERM?)

L8 0 S L5 AND (ETHYL CELLULOSE)

L9 0 S L5 AND (CELLULOSE)

L10 0 S L5 AND (GLYCEROL)

L11 1 S L4 AND (GLYCEROL OR ACNE OR CELLULOSE OR CETOMAKROGEL OR METH

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